ELSEVIER

Available online at www.sciencedirect.com

SCIENCE DIRECT®

Chemical Physics Letters 401 (2005) 597–607

CHEMICAL PHYSICS LETTERS

www.elsevier.com/locate/cplett

Author Index to Volume 401

Abe, M., see Maniwa, Y. 401 (2005) 534
Achiba, Y., see Maniwa, Y. 401 (2005) 534
Aida, M. and M. Dupuis, Fundamental absorption frequency from quasi-classical direct ab initio molecular dynamics: diatomic molecule 401 (2005) 170
Alleman, J.L., see Dillon, A.C. 401 (2005) 522
Allonas, X., see Lalevee, J. 401 (2005) 483
Allonas, X., see Szemik-Hojniak, A. 401 (2005) 189
Alonso, J.L., see Sánchez, R. 401 (2005) 259
Anandan, S., see Okazaki, M. 401 (2005) 363
Andrews, D., see Rathbone, G.J. 401 (2005) 570
Angeles Izquierdo, M., T.D.M. Bell, S. Habuchi, E. Fron, R. Pilot, T. Vosch, S. De Feyter, J. Verhoeven, J. Jacob, K. Müllen, J. Hofkens and F.C. De Schryver, Switching of the fluorescence emission of single molecules between the locally excited and charge transfer states 401 (2005) 503
Antoine, R., see Poulain, P. 401 (2005) 1
Arunima, and N.D. Kurur, Cross-correlated relaxation evidence for the intramolecular C–H···N hydrogen bond in solution 401 (2005) 470
Ault, B.S., see Goldberg, N. 401 (2005) 89

Bae, S.Y., see Kim, K.-E. 401 (2005) 459
Bagryansky, V.A., see Barlukova, M.M. 401 (2005) 62
Bakó, I., see Onthong, U. 401 (2005) 217
Balkowski, G., see Szemik-Hojniak, A. 401 (2005) 189
Balón, M., see Muñoz, M.A. 401 (2005) 109
Ban, H., see Peng, J. 401 (2005) 94
Ban, F., see Mothana, B. 401 (2005) 7
Bandow, S., T. Yamaguchi and S. Iijima, Magnetism of adsorbed oxygen on carbon nanohorns 401 (2005) 380
Bandyopadhyay, A., A. Ray, B. Ray and P.N. Ghosh, On line shape measurement and simulation of rovibrational transitions of water vapour in the near infrared region 401 (2005) 135
Banerjee, M., see Bhattacharya, S. 401 (2005) 323
Bangal, P.R., Hydrogen-bonding and protonation effects on the formation of charge transfer complex between *para*-benzoquinone and 2,6-dimethoxy phenol 401 (2005) 200
Barbatti, M., G. Granucci, M. Persico and H. Lischka, Semiempirical molecular dynamics investigation of the excited state lifetime of ethylene 401 (2005) 276
Barlukova, M.M., N.P. Gritsan, V.A. Bagryansky, V.F. Starichenko, I.A. Grigor'ev and Yu.N. Molin, OD ESR detection of the radical anions of cyclic nitrones in liquid solutions 401 (2005) 62
Barrio, M., see Puertas, R. 401 (2005) 368
Baştuğ, T. and S. Kuyucak, Memory effects in Brownian dynamics simulations of ion transport 401 (2005) 175
Bauri, A.K., see Bhattacharya, S. 401 (2005) 323
Bea, A.E., A.V. Ranea, I.M. Irurzun and E.E. Mola, Kinetics of immobile adsorption of linear molecules on a two-dimensional lattice 401 (2005) 342
Belelli, P.G., D.E. Damiani and N.J. Castellani, DFT theoretical studies of UV–Vis spectra and solvent effects in olefin polymerization catalysts 401 (2005) 515

doi:10.1016/S0009-2614(04)01968-2

Bell, T.D.M., see Angeles Izquierdo, M. 401 (2005) 503
Bhattacharya, S., A.K. Bauri, S. Chattopadhyay and M. Banerjee, Study of formation equilibria between [70]fullerene and a series of anisole by NMR spectrometric method 401 (2005) 323
Blanco, S., see Sánchez, R. 401 (2005) 259
Blau, W.J., see Nicolosi, V. 401 (2005) 13
Boatwright, A., see Curtis, S. 401 (2005) 254
Bowen Jr., K.H., see Zheng, W. 401 (2005) 266
Boyd, R.J., see Mothana, B. 401 (2005) 7
Brauer, C.S., G. Sedo, E.M. Grumstrup, K.R. Leopold, M.D. Marshall and H.O. Leung, Effects of partially quenched orbital angular momentum on the microwave spectrum and magnetic hyperfine splitting in the OH–water complex 401 (2005) 420
Broyer, M., see Poulain, P. 401 (2005) 1
Buma, W.J., see Szemik-Hojniak, A. 401 (2005) 189

Cacciani, P., see Puzzarini, C. 401 (2005) 357
Cai, M.-Q., Z. Yin, M.-S. Zhang and Y.-Z. Li, First-principles study of ferroelectric and nonlinear optical property in bismuth titanate 401 (2005) 405
Carmona, C., see Muñoz, M.A. 401 (2005) 109
Castellani, N.J., see Belelli, P.G. 401 (2005) 515
Chaban, G.M., Theoretical study of chemical compounds formed by insertion of rare gas atoms into glycine molecule: a step towards bio-ðrare gas chemistry? 401 (2005) 318
Chakrabarty, D., see Seth, D. 401 (2005) 546
Chakraborty, A., see Seth, D. 401 (2005) 546
Chao, I., see Chen, H.-Y. 401 (2005) 539
Chattopadhyay, S., see Bhattacharya, S. 401 (2005) 323
Chen, J., Z. Feng, J. Shi, P. Ying, H. Zhang and C. Li, The surface sites of sulfated zirconia studied in situ by laser-induced fluorescence spectroscopy 401 (2005) 104
Chen, Q., see Wu, M. 401 (2005) 374
Chen, H.-Y. and I. Chao, Effect of perfluorination on the charge-transport properties of organic semiconductors: density functional theory study of perfluorinated pentacene and sexithiophene 401 (2005) 539
Chen, C.-W., see Liu, H.-L. 401 (2005) 24
Chibisov, A.K., H. Görner and T.D. Slavnova, Reply to comment on 'Kinetics of salt-induced *J*-aggregation of an anionic thiacarbocyanine dye in aqueous solution' 401 (2005) 592
Cho, J.H., see Shen, G. 401 (2005) 414
Cho, J.H., see Shen, G. 401 (2005) 529
Choi, J., see Kim, K.-E. 401 (2005) 459
Choo, J., see Kim, K.-E. 401 (2005) 459
Coleman, J.N., see Nicolosi, V. 401 (2005) 13
Cong, S.-L., see Wang, S.-M. 401 (2005) 509
Cosléou, J., see Puzzarini, C. 401 (2005) 357
Cuesta, I.G., A. Ligabue, A.S. de Merás and P. Lazzeretti, The ring-current model of the paratropic pentalene molecule 401 (2005) 282
Cundari, T.R., H.A.R. Leza, T. Grimes, G. Steyl, A. Waters and A.K. Wilson, Calculation of the enthalpies of formation for transition metal complexes 401 (2005) 58
Curtis, S., A. Boatwright, R.R. Wright and A.J. Stace, Evidence of a shift between one- and two-photon processes associated with benzene trapped in helium nanodroplets 401 (2005) 254

Damiani, D.E., see Belelli, P.G. 401 (2005) 515
Dang, Z.-M., see Zhang, Y.-H. 401 (2005) 553
Das, K., B. Jain, A. Dube and P.K. Gupta, pH dependent binding of chlorin-p6 with phosphatidyl choline liposomes 401 (2005) 185
De Feyter, S., see Angeles Izquierdo, M. 401 (2005) 503
de la Fuente, M.R., see Puertas, R. 401 (2005) 368
de Merás, A.S., see Cuesta, I.G. 401 (2005) 282
De Schryver, F.C., see Angeles Izquierdo, M. 401 (2005) 503
Deng, J.-G., see Zhang, Y.-H. 401 (2005) 553

Deng, J.K., see Zhang, S.F. 401 (2005) 80
Denifl, S., see Ptasińska, S. 401 (2005) 227
Deperasińska, I., see Szemik-Hojniak, A. 401 (2005) 189
Diez, S., see Puertas, R. 401 (2005) 368
DiLabio, G.A., see Johnson, E.R. 401 (2005) 595
Dillon, A.C., P.A. Parilla, J.L. Alleman, T. Gennett, K.M. Jones and M.J. Heben, Systematic inclusion of defects in pure carbon single-wall nanotubes and their effect on the Raman D-band 401 (2005) 522
Ding, T., see Tian, H.W. 401 (2005) 585
Djurišic, A.B., see Xiangfeng, C. 401 (2005) 426
Dongli, J., see Xiangfeng, C. 401 (2005) 426
Douhal, A., see Sanz, M. 401 (2005) 435
Dreyer, J., see Usman, A. 401 (2005) 157
Duan, W., see Hao, S. 401 (2005) 47
Dube, A., see Das, K. 401 (2005) 185
Dugourd, P., see Poulain, P. 401 (2005) 1
Dunne, L.J., see Manos, G. 401 (2005) 430
Dunsch, L., see Petr, A. 401 (2005) 130
Dupuis, M., see Aida, M. 401 (2005) 170

Efremenko, I. and M. Sheintuch, DFT study of small bimetallic palladium–copper clusters 401 (2005) 232
Egdell, R.G., see Lynch, C.C.B. 401 (2005) 223
El-Gezawy, H., W. Rettig and R. Lapouyade, Model studies of spectral and photophysical characteristics of donor-acceptor-polyenes: dimethylamino-cyano-diphenylbutadiene 401 (2005) 140
Eriksson, L.A., see Li, X. 401 (2005) 99

Fang, J., C. Zhong and R. Mu, The study of deposited silver particulate films by simple method for efficient SERS 401 (2005) 271
Feng, Z., see Chen, J. 401 (2005) 104
Fouassier, J.P., see Lalevee, J. 401 (2005) 483
Fowler, P.W., see Soncini, A. 401 (2005) 164
Fritzsche, S., see Uvarov, A. 401 (2005) 296
Fron, E., see Angeles Izquierdo, M. 401 (2005) 503
Fu, S.-Y., see Zhang, Y.-H. 401 (2005) 553

Galán, M., see Muñoz, M.A. 401 (2005) 109
Gao, Y., see Magyar, R.J. 401 (2005) 149
Gao, F., see Mei, E. 401 (2005) 30
García-Río, L., A. Godoy and J.R. Leis, Spectroscopic characterisation of crystal violet inclusion complexes in β-cyclodextrin 401 (2005) 302
García-Revilla, S., P. Gerner, O.S. Wenger, H.U. Güdel and R. Valiente, Visible Ni^{2+} upconversion luminescence in Ni^{2+}, Yb^{3+} co-doped $CsCdBr_3$ 401 (2005) 492
Geerlings, P., see Mignon, P. 401 (2005) 40
Gennett, T., see Dillon, A.C. 401 (2005) 522
Gerner, P., see García-Revilla, S. 401 (2005) 492
Ghosh, P.N., see Bandyopadhyay, A. 401 (2005) 135
Godoy, A., see García-Río, L. 401 (2005) 302
Goldberg, N. and B.S. Ault, Electronic spectra of intermediate charge transfer complexes of $OVCl_3$ in argon matrices 401 (2005) 89
Görner, H., see Chibisov, A.K. 401 (2005) 592
Granucci, G., see Barbatti, M. 401 (2005) 276
Grigor'ev, I.A., see Barlukova, M.M. 401 (2005) 62
Grimes, T., see Cundari, T.R. 401 (2005) 58
Gritsan, N.P., see Barlukova, M.M. 401 (2005) 62
Grumstrup, E.M., see Brauer, C.S. 401 (2005) 420
Gu, B.-L., see Hao, S. 401 (2005) 47
Güdel, H.U., see García-Revilla, S. 401 (2005) 492

Gueorguiev, G.K., J. Neidhardt, S. Stafström and L. Hultman, First-principles calculations on the role of CN precursors for the formation of fullerene-like carbon nitride 401 (2005) 288
Guo, Z.-X., see Hu, J. 401 (2005) 352
Gupta, P.K., see Das, K. 401 (2005) 185

Habuchi, S., see Angeles Izquierdo, M. 401 (2005) 503
Haneda, H., see Li, D. 401 (2005) 579
Hanoune, B. and B. Lemoine, Frequency stabilization of tunable infrared diode lasers for time-resolved monitoring of transient species 401 (2005) 180
Hansen, Aa.E., see Kongsted, J. 401 (2005) 385
Hao, S., G. Zhou, J. Wu, W. Duan and B.-L. Gu, Spin-polarized electron current from Mn-doped closed zigzag GaN nanotubes 401 (2005) 47
Hättig, C., see Kongsted, J. 401 (2005) 385
Heben, M.J., see Dillon, A.C. 401 (2005) 522
Herlemont, F., see Puzzarini, C. 401 (2005) 357
Hermansson, K., see Onthong, U. 401 (2005) 217
Herricks, T., see Im, S.H. 401 (2005) 19
Heyne, K., see Usman, A. 401 (2005) 157
Higo, J., see Yokomizo, T. 401 (2005) 332
Higo, J., see Kamiya, N. 401 (2005) 312
Hishita, S., see Li, D. 401 (2005) 579
Ho, Y., see Liu, H.-L. 401 (2005) 24
Hochstrasser, R.M., see Mei, E. 401 (2005) 30
Hofkens, J., see Angeles Izquierdo, M. 401 (2005) 503
Horii, F., see Kaji, H. 401 (2005) 246
Horváth, D., see Virányi, Z. 401 (2005) 575
Hou, Z., see Wang, Z. 401 (2005) 307
Hu, J., J. Shi, S. Li, Y. Qin, Z.-X. Guo, Y. Song and D. Zhu, Efficient method to functionalize carbon nanotubes with thiol groups and fabricate gold nanocomposites 401 (2005) 352
Huang, F., see Zhang, S.F. 401 (2005) 80
Hultman, L., see Gueorguiev, G.K. 401 (2005) 288

Iijima, S., see Bandow, S. 401 (2005) 380
Ikegami, K., Comment on 'Kinetics of salt-induced *J*-aggregation of anionic thiacarbocyanine dye in aqueous solution' [Chem. Phys. Lett. 390 (2004) 240] 401 (2005) 590
Ikejiri, K., H. Ohoyama, Y. Nagamachi and T. Kasai, A highly intense state-selected CH radical beam and its application to the CH + O_2 reaction 401 (2005) 465
Ikeuchi, S., see Saito, K. 401 (2005) 76
Im, S.H., T. Herricks, Y.T. Lee and Y. Xia, Synthesis and characterization of monodisperse silica colloids loaded with superparamagnetic iron oxide nanoparticles 401 (2005) 19
Irurzun, I.M., see Bea, A.E. 401 (2005) 342
Ishida, T., see Tamura, H. 401 (2005) 487
Ishikawa, Y., see Takahashi, M. 401 (2005) 475
Ito, H., see Takahashi, M. 401 (2005) 475

Jacob, J., see Angeles Izquierdo, M. 401 (2005) 503
Jacobson, M.L. and K.L. Rowlen, Photo-dynamics on thin silver films 401 (2005) 52
Jain, B., see Das, K. 401 (2005) 185
Jalili, S.E., see Manos, G. 401 (2005) 430
Janczyk, A., S.K. Walter and L.M. Ziurys, Examining the transition metal hydrosulfides: the pure rotational spectrum of CuSH ($\tilde{X}^1A'$) 401 (2005) 211
Jia, Y., see Wu, M. 401 (2005) 374
Jiang, Q., see Tian, H.W. 401 (2005) 585
Johnson, E.R., R.A. Wolkow and G.A. DiLabio, Reply to comment on 'Application of 25 density functionals to dispersion-bound homomolecular dimers' [Chem. Phys. Lett. 394 (2004) 334–338] 401 (2005) 595
Jones, K.M., see Dillon, A.C. 401 (2005) 522

Jørgensen, P., see Kongsted, J. 401 (2005) 385
Jung, W.S., see Kim, K.-E. 401 (2005) 459
Jung, S.I., see Shen, G. 401 (2005) 529

Kadowaki, H., see Maniwa, Y. 401 (2005) 534
Kaji, H., T. Yamada, N. Tsukamoto and F. Horii, A combined experimental and theoretical study of the conformation of *N*,*N*′-diphenyl-*N*,*N*′-di(*m*-tolyl)benzidine using solid-state ^{15}N NMR and DFT calculations 401 (2005) 246
Kamiya, N., Y.S. Watanabe, S. Ono and J. Higo, AMBER-based hybrid force field for conformational sampling of polypeptides 401 (2005) 312
Kasai, T., see Ikejiri, K. 401 (2005) 465
Kataura, H., see Maniwa, Y. 401 (2005) 534
Kaziannis, S., P. Siozos and C. Kosmidis, Dynamic alignment of CH_3I by strong picosecond laser pulses 401 (2005) 115
Khan, A., Solvated electron in $(H_2O)_{20}^-$ dodecahedral cavity: calculated stretch frequencies and vertical dissociation energy 401 (2005) 85
Khelkhal, M., see Puzzarini, C. 401 (2005) 357
Kim, K.-E., K.-J. Kim, W.S. Jung, S.Y. Bae, J. Park, J. Choi and J. Choo, Investigation on the temperature-dependent growth rate of carbon nanotubes using chemical vapor deposition of ferrocene and acetylene 401 (2005) 459
Kim, K.-J., see Kim, K.-E. 401 (2005) 459
Kira, H., see Maniwa, Y. 401 (2005) 534
Kjellberg, P., see Sun, M. 401 (2005) 558
Kongsted, J., T.B. Pedersen, M. Strange, A. Osted, Aa.E. Hansen, K.V. Mikkelsen, F. Pawlowski, P. Jørgensen and C. Hättig, Coupled cluster calculations of the optical rotation of *S*-propylene oxide in gas phase and solution 401 (2005) 385
Kosmidis, C., see Kaziannis, S. 401 (2005) 115
Kotaidis, V., see Plech, A. 401 (2005) 565
Kunimatsu, K., T. Senzaki, M. Tsushima and M. Osawa, A combined surface-enhanced infrared and electrochemical kinetics study of hydrogen adsorption and evolution on a Pt electrode 401 (2005) 451
Kurur, N.D., see Arunima, 401 (2005) 470
Kuyucak, S., see Baştuğ, T. 401 (2005) 175

Labhsetwar, N.K., see Li, D. 401 (2005) 579
Lalevee, J., X. Allonas and J.P. Fouassier, Triplet–triplet energy transfer reaction to *cis*-stilbene: a dual thermal bond activation mechanism 401 (2005) 483
Lapouyade, R., see El-Gezawy, H. 401 (2005) 140
Law, D.S.L., see Lynch, C.C.B. 401 (2005) 223
Lawrance, W.D., see Sampson, R.K. 401 (2005) 440
Lazzeretti, P., see Soncini, A. 401 (2005) 164
Lazzeretti, P., see Cuesta, I.G. 401 (2005) 282
Lee, C.J., see Shen, G. 401 (2005) 414
Lee, Y.T., see Im, S.H. 401 (2005) 19
Lee, C.J., see Shen, G. 401 (2005) 529
Leis, J.R., see García-Río, L. 401 (2005) 302
Lemoine, B., see Hanoune, B. 401 (2005) 180
Leopold, K.R., see Brauer, C.S. 401 (2005) 420
Lesarri, A., see Sánchez, R. 401 (2005) 259
Leung, Y.H., see Xiangfeng, C. 401 (2005) 426
Leung, H.O., see Brauer, C.S. 401 (2005) 420
Leza, A.R.H., see Cundari, T.R. 401 (2005) 58
Li, S., see Hu, J. 401 (2005) 352
Li, X. and L.A. Eriksson, Influence of C5-methylation of cytosine on the formation of cyclobutane pyrimidine dimers 401 (2005) 99
Li, X.T., see Tian, H.W. 401 (2005) 585
Li, G.Q., see Zhang, S.F. 401 (2005) 80

Li, D., H. Haneda, N.K. Labhsetwar, S. Hishita and N. Ohashi, Visible-light-driven photocatalysis on fluorine-doped TiO_2 powders by the creation of surface oxygen vacancies 401 (2005) 579
Li, L.-F., see Zhang, Y.-H. 401 (2005) 553
Li, B., see Zhang, S.F. 401 (2005) 80
Li, Y.-Z., see Cai, M.-Q. 401 (2005) 405
Li, C., see Chen, J. 401 (2005) 104
Liao, B., A 2D graphical representation of DNA sequence 401 (2005) 196
Ligabue, A., see Cuesta, I.G. 401 (2005) 282
Limão-Vieira, P., see Ptasińska, S. 401 (2005) 227
Lin, J.-C., see Liu, H.-L. 401 (2005) 24
Lineberger, W.C., see Rathbone, G.J. 401 (2005) 570
Lischka, H., see Barbatti, M. 401 (2005) 276
Liu, H.-L., J.-C. Lin, Y. Ho and C.-W. Chen, Homology models of main proteinase from coronavirus associated with SARS 401 (2005) 24
López, D.O., see Puertas, R. 401 (2005) 368
López, J.C., see Sánchez, R. 401 (2005) 259
Lórenc, M., see Plech, A. 401 (2005) 565
Loverix, S., see Mignon, P. 401 (2005) 40
Lundberg, M. and P.E.M. Siegbahn, Minimum energy spin crossings for an O–O bond formation reaction 401 (2005) 347
Lynch, C.C.B., R.G. Egdell and D.S.L. Law, High resolution X-ray photoemission of $SrCu_2O_2$ 401 (2005) 223

Ma, F., see Sun, M. 401 (2005) 558
Magyar, R.J., S. Tretiak, Y. Gao, H.-L. Wang and A.P. Shreve, A joint theoretical and experimental study of phenylene–acetylene molecular wires 401 (2005) 149
Maniwa, Y., H. Kataura, M. Abe, A. Udaka, S. Suzuki, Y. Achiba, H. Kira, K. Matsuda, H. Kadowaki and Y. Okabe, Ordered water inside carbon nanotubes: formation of pentagonal to octagonal ice-nanotubes 401 (2005) 534
Manos, G., L.J. Dunne and S.E. Jalili, Matrix computation of the statistical mechanics of a lattice model of multistep benzene adsorption isotherms in silicalite 401 (2005) 430
Märk, T.D., see Ptasińska, S. 401 (2005) 227
Marshall, M.D., see Brauer, C.S. 401 (2005) 420
Mashiko, S., see Okuno, Y. 401 (2005) 35
Matsuda, K., see Maniwa, Y. 401 (2005) 534
McCauley, J., see Nicolosi, V. 401 (2005) 13
Megyes, T., see Onthong, U. 401 (2005) 217
Mei, E., F. Gao, S. Vinogradov, J.M. Vanderkooi and R.M. Hochstrasser, Phosphorescence of individual horseradish peroxidases proteins having a modified heme group 401 (2005) 30
Meier, R.J., Comment on 'Application of 25 density functionals to dispersion-bound homomolecular dimers' by Johnson, Wolkow and DiLabio, Chem. Phys. Lett. 394 (2004) 334–338 401 (2005) 594
Meijerink, A., see Peijzel, P.S. 401 (2005) 241
Meng, F.L., see Tian, H.W. 401 (2005) 585
Mignon, P., S. Loverix and P. Geerlings, Interplay between π–π interactions and the H-bonding ability of aromatic nitrogen bases 401 (2005) 40
Mihailovic, D., see Nicolosi, V. 401 (2005) 13
Mikkelsen, K.V., see Kongsted, J. 401 (2005) 385
Moc, J., Reactivity of aluminium dimer with H_2: the performance of high level ab initio and density functional methods for prediction of reaction paths 401 (2005) 497
Mohammed, O.F., see Usman, A. 401 (2005) 157
Mola, E.E., see Bea, A.E. 401 (2005) 342
Molin, Yu.N., see Barlukova, M.M. 401 (2005) 62
Morgan, M., see Tuchler, M.F. 401 (2005) 393
Mothana, B., F. Ban and R.J. Boyd, Validation of a computational scheme to study ^{15}N and ^{13}C nuclear shielding constants 401 (2005) 7
Mrzel, A., see Nicolosi, V. 401 (2005) 13
Mu, R., see Fang, J. 401 (2005) 271

Mukai, K., see Saito, K. 401 (2005) 122
Mukherjee, B. and A.J. Pal, Dielectric properties of (multilevel) switching devices based on ultrathin organic films 401 (2005) 410
Mukherjee, A.K., see Ray, A.K. 401 (2005) 72
Müllen, K., see Angeles Izquierdo, M. 401 (2005) 503
Muñoz, M.A., M. Galán, C. Carmona and M. Balón, Hydrogen-bonding interactions between 1-methylindole and alcohols 401 (2005) 109

Nagamachi, Y., see Ikejiri, K. 401 (2005) 465
Nakamura, H., see Tamura, H. 401 (2005) 487
Nakasako, M., see Yokomizo, T. 401 (2005) 332
Nanbu, S., see Tamura, H. 401 (2005) 487
Neidhardt, J., see Gueorguiev, G.K. 401 (2005) 288
Neudeck, A., see Petr, A. 401 (2005) 130
Nguyen, M.T., see Oláh, J. 401 (2005) 337
Nibbering, E.T.J., see Usman, A. 401 (2005) 157
Nicolosi, V., D. Vrbanic, A. Mrzel, J. McCauley, S. O'Flaherty, D. Mihailovic, W.J. Blau and J.N. Coleman, Solubility of $Mo_6S_{4.5}I_{4.5}$ nanowires 401 (2005) 13
Nilles, J.M., see Zheng, W. 401 (2005) 266
Ning, C.G., see Zhang, S.F. 401 (2005) 80
Nishizawa, J., see Takahashi, M. 401 (2005) 475
Niu, H., see Wu, M. 401 (2005) 374

O'Flaherty, S., see Nicolosi, V. 401 (2005) 13
Ohashi, N., see Li, D. 401 (2005) 579
Ohoyama, H., see Ikejiri, K. 401 (2005) 465
Okabe, Y., see Maniwa, Y. 401 (2005) 534
Okazaki, M., K. Toriyama and S. Anandan, Dynamics and packing mode of long-chained *n*-alkane molecules in the nano-channel of MCM-41 401 (2005) 363
Okuno, Y. and S. Mashiko, Fast computation algorithm for finding stable molecular structures using network-connected computers 401 (2005) 35
Oláh, J., T. Veszprémi and M.T. Nguyen, Spin-philicity and spin-donicity of simple nitrenes and phosphinidenes 401 (2005) 337
Ono, S., see Kamiya, N. 401 (2005) 312
Onthong, U., T. Megyes, I. Bakó, T. Radnai, K. Hermansson and M. Probst, Molecular dynamics simulation of lithium iodide in liquid dimethylsulfoxide 401 (2005) 217
Osawa, M., see Kunimatsu, K. 401 (2005) 451
Osted, A., see Kongsted, J. 401 (2005) 385
Ota, A., see Saito, K. 401 (2005) 76

Pal, A.J., see Mukherjee, B. 401 (2005) 410
Pal, P., see Sarkar, J. 401 (2005) 400
Pardo, L.C., see Puertas, R. 401 (2005) 368
Parilla, P.A., see Dillon, A.C. 401 (2005) 522
Park, J., see Kim, K.-E. 401 (2005) 459
Pawlowski, F., see Kongsted, J. 401 (2005) 385
Pedersen, T.B., see Kongsted, J. 401 (2005) 385
Peijzel, P.S. and A. Meijerink, Visible photon cascade emission from the high energy levels of Er^{3+} 401 (2005) 241
Peng, J., H. Ban, X. Zhang, L. Song and Z. Sun, Binary adsorption equilibrium of propylene and ethylene on silicalite-1: prediction and experiment 401 (2005) 94
Persico, M., see Barbatti, M. 401 (2005) 276
Pérez-Jubindo, M.A., see Puertas, R. 401 (2005) 368
Persky, A., The rate constants of the two channels of the reaction of F atoms with HD in the temperature range 193–300 K 401 (2005) 455
Petr, A., A. Neudeck and L. Dunsch, On the magnetic susceptibility of polyaniline – an alternative approach 401 (2005) 130

Pilot, R., see Angeles Izquierdo, M. 401 (2005) 503
Plech, A., V. Kotaidis, M. Lorenc and M. Wulff, Thermal dynamics in laser excited metal nanoparticles 401 (2005) 565
Poulain, P., R. Antoine, M. Broyer and P. Dugourd, Monte Carlo simulations of flexible molecules in a static electric field: electric dipole and conformation 401 (2005) 1
Pozharskii, A.F., see Szemik-Hojniak, A. 401 (2005) 189
Probst, M., see Onthong, U. 401 (2005) 217
Ptasińska, S., P. Limão-Vieira, S. Denifl, P. Scheier and T.D. Märk, Electron attachment to monomeric and dimeric forms of glycolaldehyde 401 (2005) 227
Puertas, R., J. Salud, D.O. López, M.A. Rute, S. Diez, J.Ll. Tamarit, M. Barrio, M.A. Pérez-Jubindo, M.R. de la Fuente and L.C. Pardo, Static and dynamic studies on cycloheptanol as two-orientational glass-former 401 (2005) 368
Pullerits, T., see Sun, M. 401 (2005) 558
Puzzarini, C., J. Cosléou, P. Cacciani, F. Herlemont and M. Khelkhal, CH_3F: the magnetic interactions at the origin of the nuclear spin conversion 401 (2005) 357

Qi, H., see Wu, M. 401 (2005) 374
Qin, Y., see Hu, J. 401 (2005) 352

Radnai, T., see Onthong, U. 401 (2005) 217
Randić, M., see Vukičević, D. 401 (2005) 446
Ranea, A.V., see Bea, A.E. 401 (2005) 342
Rathbone, G.J., T. Sanford, D. Andrews and W.C. Lineberger, Photoelectron imaging spectroscopy of $Cu^-(H_2O)_{1,2}$ anion complexes 401 (2005) 570
Ray, B., see Bandyopadhyay, A. 401 (2005) 135
Ray, A., see Bandyopadhyay, A. 401 (2005) 135
Ray, A.K., A. Saha and A.K. Mukherjee, A partition experimental evidence of molecular complex formation of some quinones with sodium dodecyl sulphate anion in aqueous phase by spectrophotometric method 401 (2005) 72
Ren, X.G., see Zhang, S.F. 401 (2005) 80
Rettig, W., see El-Gezawy, H. 401 (2005) 140
Rowlen, K.L., see Jacobson, M.L. 401 (2005) 52
Rute, M.A., see Puertas, R. 401 (2005) 368

Saha, A., see Ray, A.K. 401 (2005) 72
Saito, K., S. Ikeuchi, A. Ota, H. Yamochi and G. Saito, Entropic evidence for cooperation of multiple instabilities upon a metal–insulator transition in $(EDO\text{-}TTF)_2PF_6$ 401 (2005) 76
Saito, K., K. Mukai and H. Sumi, Excited states of pigments in photosystem II reaction centers of photosynthesis: Characterization into a central dimer and remaining monomers 401 (2005) 122
Saito, G., see Saito, K. 401 (2005) 76
Salud, J., see Puertas, R. 401 (2005) 368
Sampson, R.K. and W.D. Lawrance, Bound orbiting states of benzene–Ar and evidence for reversible intramolecular vibrational energy redistribution within the complex 401 (2005) 440
Sánchez, R., S. Blanco, A. Lesarri, J.C. López and J.L. Alonso, The rotational spectrum of the 3,3-dimethyloxetane···hydrogen chloride complex 401 (2005) 259
Sanford, T., see Rathbone, G.J. 401 (2005) 570
Sanz, M. and A. Douhal, Femtosecond emission study of H-atom transfer reaction dynamics in a new system with an internal H-bond 401 (2005) 435
Sarkar, J., P. Pal and G.B. Talapatra, Self-assembly of silver nano-particles on stearic acid Langmuir–Blodgett film: evidence of fractal growth 401 (2005) 400
Sarkar, N., see Seth, D. 401 (2005) 546
Saven, J.G., see Yang, X. 401 (2005) 205
Scheier, P., see Ptasińska, S. 401 (2005) 227
Schmidt, K.L., see Tuchler, M.F. 401 (2005) 393
Sedo, G., see Brauer, C.S. 401 (2005) 420
Senzaki, T., see Kunimatsu, K. 401 (2005) 451

Seth, D., D. Chakrabarty, A. Chakraborty and N. Sarkar, Study of energy transfer from 7-amino coumarin donors to rhodamine 6G acceptor in non-aqueous reverse micelles 401 (2005) 546
Sheintuch, M., see Efremenko, I. 401 (2005) 232
Shen, G., J.H. Cho and C.J. Lee, Morphology-controlled synthesis, growth mechanism and optical properties of ZnO nanonails 401 (2005) 414
Shen, G., J.H. Cho, S.I. Jung and C.J. Lee, Synthesis and characterization of S-doped ZnO nanowires produced by a simple solution-conversion process 401 (2005) 529
Shi, J., see Chen, J. 401 (2005) 104
Shi, J., see Hu, J. 401 (2005) 352
Shindo, H., see Yokomizo, T. 401 (2005) 332
Shreve, A.P., see Magyar, R.J. 401 (2005) 149
Siegbahn, P.E.M., see Lundberg, M. 401 (2005) 347
Siozos, P., see Kaziannis, S. 401 (2005) 115
Slavnova, T.D., see Chibisov, A.K. 401 (2005) 592
Soncini, A., P.W. Fowler, P. Lazzeretti and R. Zanasi, Ring-current signatures in shielding-density maps 401 (2005) 164
Song, Y., see Hu, J. 401 (2005) 352
Song, L., see Peng, J. 401 (2005) 94
Stace, A.J., see Curtis, S. 401 (2005) 254
Stafström, S., see Gueorguiev, G.K. 401 (2005) 288
Starichenko, V.F., see Barlukova, M.M. 401 (2005) 62
Steyl, G., see Cundari, T.R. 401 (2005) 58
Strange, M., see Kongsted, J. 401 (2005) 385
Su, G.L., see Zhang, S.F. 401 (2005) 80
Sumi, H., see Saito, K. 401 (2005) 122
Sun, M., P. Kjellberg, F. Ma and T. Pullerits, Excited state properties of acceptor-substitute carotenoids: 2D and 3D real-space analysis 401 (2005) 558
Sun, Z., see Peng, J. 401 (2005) 94
Suzuki, S., see Maniwa, Y. 401 (2005) 534
Szemik-Hojniak, A., I. Deperasińska, W.J. Buma, G. Balkowski, A.F. Pozharskii, N.V. Vistorobskii and X. Allonas, The asymmetric nature of charge transfer states of the cyano-substituted proton sponge 401 (2005) 189

Takahashi, M., Y. Ishikawa, J. Nishizawa and H. Ito, Low-frequency vibrational modes of riboflavin and related compounds 401 (2005) 475
Talapatra, G.B., see Sarkar, J. 401 (2005) 400
Tamarit, J.Ll., see Puertas, R. 401 (2005) 368
Tamura, H., S. Nanbu, H. Nakamura and T. Ishida, A theoretical study of cyclohexadiene/hexatriene photochemical interconversion: multireference configuration interaction potential energy surfaces and transition probabilities for the radiationless decays 401 (2005) 487
Thomas, O.C., see Zheng, W. 401 (2005) 266
Tian, H.W., W.T. Zheng, Z.D. Zhao, T. Ding, S.S. Yu, B. Zheng, X.T. Li, F.L. Meng and Q. Jiang, Magnetic properties and electron spin resonance of charge ordering manganite $Y_{0.5}Ca_{0.5}MnO_3$ 401 (2005) 585
Toriyama, K., see Okazaki, M. 401 (2005) 363
Tóth, Á., see Virányi, Z. 401 (2005) 575
Tretiak, S., see Magyar, R.J. 401 (2005) 149
Tsukamoto, N., see Kaji, H. 401 (2005) 246
Tsushima, S. and T. Yang, Relativistic density functional theory study on the structure and bonding of U(IV) and Np(IV) hydrates 401 (2005) 68
Tsushima, M., see Kunimatsu, K. 401 (2005) 451
Tuchler, M.F., K.L. Schmidt and M. Morgan, A CRDS approach to gas phase equilibrium constants: the case of $N_2O_4 \leftrightarrow 2NO_2$ at 283 K 401 (2005) 393

Udaka, A., see Maniwa, Y. 401 (2005) 534
Usman, A., O.F. Mohammed, K. Heyne, J. Dreyer and E.T.J. Nibbering, Excited state dynamics of a PYP chromophore model system explored with ultrafast infrared spectroscopy 401 (2005) 157

Uvarov, A. and S. Fritzsche, A semi-phenomenological approach to the transport and diffusion of small spherical macromolecules in solution 401 (2005) 296

Valiente, R., see García-Revilla, S. 401 (2005) 492
Vanderkooi, J.M., see Mei, E. 401 (2005) 30
Verhoeven, J., see Angeles Izquierdo, M. 401 (2005) 503
Veszprémi, T., see Oláh, J. 401 (2005) 337
Vinogradov, S., see Mei, E. 401 (2005) 30
Virányi, Z., Á. Tóth and D. Horváth, Lateral instability induced by an inhomogeneous electric field 401 (2005) 575
Vistorobskii, N.V., see Szemik-Hojniak, A. 401 (2005) 189
Vosch, T., see Angeles Izquierdo, M. 401 (2005) 503
Vrbanic, D., see Nicolosi, V. 401 (2005) 13
Vukičević, D. and M. Randić, On Kekulé structures of buckminsterfullerene 401 (2005) 446

Walter, S.K., see Janczyk, A. 401 (2005) 211
Wang, H.-L., see Magyar, R.J. 401 (2005) 149
Wang, Z., Z. Hou and H. Xin, Internal noise stochastic resonance of synthetic gene network 401 (2005) 307
Wang, S.-M., S.-L. Cong, K.-J. Yuan and J. Yu, Probing wave packet dynamics of $B^2\Pi$ and $C^2\Pi$ states of NO molecule with time- and energy-resolved photoelectron spectra 401 (2005) 509
Watanabe, Y.S., see Kamiya, N. 401 (2005) 312
Waters, A., see Cundari, T.R. 401 (2005) 58
Wenger, O.S., see García-Revilla, S. 401 (2005) 492
Wilson, A.K., see Cundari, T.R. 401 (2005) 58
Wolkow, R.A., see Johnson, E.R. 401 (2005) 595
Wright, R.R., see Curtis, S. 401 (2005) 254
Wu, J., see Zhang, Y.-H. 401 (2005) 553
Wu, J., see Hao, S. 401 (2005) 47
Wu, M., Y. Xiong, Y. Jia, H. Niu, H. Qi, J. Ye and Q. Chen, Magnetic field-assisted hydrothermal growth of chain-like nanostructure of magnetite 401 (2005) 374
Wulff, M., see Plech, A. 401 (2005) 565

Xia, Y., see Im, S.H. 401 (2005) 19
Xiangfeng, C., J. Dongli, A.B. Djurišic and Y.H. Leung, Gas-sensing properties of thick film based on ZnO nano-tetrapods 401 (2005) 426
Xin, J.H., see Zhang, Y.-H. 401 (2005) 553
Xin, H., see Wang, Z. 401 (2005) 307
Xiong, Y., see Wu, M. 401 (2005) 374

Yamada, T., see Kaji, H. 401 (2005) 246
Yamaguchi, T., see Bandow, S. 401 (2005) 380
Yamazaki, T., see Yokomizo, T. 401 (2005) 332
Yamochi, H., see Saito, K. 401 (2005) 76
Yan, Q., see Zhang, Y.-H. 401 (2005) 553
Yang, X. and J.G. Saven, Computational methods for protein design and protein sequence variability: biased Monte Carlo and replica exchange 401 (2005) 205
Yang, S., see Zhang, Y.-H. 401 (2005) 553
Yang, T., see Tsushima, S. 401 (2005) 68
Ye, J., see Wu, M. 401 (2005) 374
Yin, Z., see Cai, M.-Q. 401 (2005) 405
Ying, P., see Chen, J. 401 (2005) 104
Yokomizo, T., M. Nakasako, T. Yamazaki, H. Shindo and J. Higo, Hydrogen-bond patterns in the hydration structure of a protein 401 (2005) 332
Yu, J., see Wang, S.-M. 401 (2005) 509
Yu, S.S., see Tian, H.W. 401 (2005) 585
Yuan, K.-J., see Wang, S.-M. 401 (2005) 509

Zanasi, R., see Soncini, A. 401 (2005) 164
Zhang, Y.-H., Z.-M. Dang, S.-Y. Fu, J.H. Xin, J.-G. Deng, J. Wu, S. Yang, L.-F. Li and Q. Yan, Dielectric and dynamic mechanical properties of polyimide–clay nanocomposite films 401 (2005) 553
Zhang, X., see Peng, J. 401 (2005) 94
Zhang, S.F., X.G. Ren, G.L. Su, C.G. Ning, H. Zhou, B. Li, F. Huang, G.Q. Li and J.K. Deng, The outer valence orbital momentum profiles of thiophene by electron momentum spectroscopy 401 (2005) 80
Zhang, H., see Chen, J. 401 (2005) 104
Zhang, M.-S., see Cai, M.-Q. 401 (2005) 405
Zhao, Z.D., see Tian, H.W. 401 (2005) 585
Zheng, B., see Tian, H.W. 401 (2005) 585
Zheng, W.T., see Tian, H.W. 401 (2005) 585
Zheng, W., J.M. Nilles, O.C. Thomas and K.H. Bowen Jr., Photoelectron spectroscopy of titanium–benzene cluster anions 401 (2005) 266
Zhong, C., see Fang, J. 401 (2005) 271
Zhou, G., see Hao, S. 401 (2005) 47
Zhou, H., see Zhang, S.F. 401 (2005) 80
Zhu, D., see Hu, J. 401 (2005) 352
Ziurys, L.M., see Janczyk, A. 401 (2005) 211